09/728,616

Welcome to STN International! Enter x:x

LOGINID:ssspta1600txm

PASSWORD:

* * * * * RECONNECTED TO STN INTERNATIONAL * * * * * * * SESSION RESUMED IN FILE 'REGISTRY' AT 17:29:12 ON 05 FEB 2004 FILE 'REGISTRY' ENTERED AT 17:29:12 ON 05 FEB 2004 COPYRIGHT (C) 2004 American Chemical Society (ACS)

COST IN U.S. DOLLARS

SINCE FILE TOTAL ENTRY SESSION 3.36 3.57

FULL ESTIMATED COST

=>

Uploading C:\Program Files\Stnexp\Queries\09728616a.str

=>

Uploading C:\Program Files\Stnexp\Queries\09728616b.str

L1 STRUCTURE UPLOADED

=> d 11

L1 HAS NO ANSWERS

L1

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

STR

Structure attributes must be viewed using STN Express query preparation.

=> s l1 exact sam

STRUCTURES CONTAINING VARIABLE NODES NOT VALID IN EXACT OR FAMILY SEARCH You have requested a full structure (EXA or FAM) search on a structure containing one of the special variable-atom symbols A, M, Q, or X, or a variable group G. Only bond variability is allowed in structures for EXA or FAM searches. Variable nodes are never permitted.

=> s l1 fam sam

STRUCTURES CONTAINING VARIABLE NODES NOT VALID IN EXACT OR FAMILY SEARCH You have requested a full structure (EXA or FAM) search on a structure containing one of the special variable-atom symbols A, M, Q, or X, or a variable group G. Only bond variability is allowed in structures for EXA or FAM searches. Variable nodes are never permitted.

=> s l1 substructure sam

COMBINATION OF STRUCTURE AND TEXT TERMS NOT VALID

The query entered contains both search terms created by structure-building or screen commands and text search terms. L#s created via the STRUCTURE or SCREEN commands must be searched in the structures files separately from text terms or profiles. The L# answer sets from structure searches can be used in crossover searches

=> s l1 sub sam ENTER SUBSET L# OR (END):l1 L1 MAY NOT BE USED HERE

and can be combined with text terms.

10/039/33

The L-number must have been created by a search in this file. To see all L-numbers defined in this session, enter DISPLAY HISTORY at an arrow prompt (=>). For additional information on subset searching in this file, enter HELP SUBSET. ENTER SUBSET L# OR (END):end SEARCH ENDED BY USER

=> s 11 sam

SAMPLE SEARCH INITIATED 17:34:00 FILE 'REGISTRY' SAMPLE SCREEN SEARCH COMPLETED -15 TO ITERATE

100.0% PROCESSED

15 ITERATIONS

1 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:

ONLINE **COMPLETE**

BATCH

COMPLETE

PROJECTED ITERATIONS:

68 TO 532

PROJECTED ANSWERS:

1 TO 80

L2

1 SEA SSS SAM L1

=> d scan str

1 ANSWERS L2REGISTRY COPYRIGHT 2004 ACS on STN

Absolute stereochemistry.

ALL ANSWERS HAVE BEEN SCANNED

=> d cost

COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
CONNECT CHARGES	6.84	6.99
NETWORK CHARGES	1.14	1.20
FULL ESTIMATED COST	7.98	8.19

IN FILE 'REGISTRY' AT 17:35:31 ON 05 FEB 2004

=> d his

(FILE 'HOME' ENTERED AT 17:23:02 ON 05 FEB 2004)

FILE 'REGISTRY' ENTERED AT 17:23:32 ON 05 FEB 2004

L1 STRUCTURE UPLOADED

L2 1 S L1 SAM

=> s l1 full

FULL SEARCH INITIATED 17:36:52 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 365 TO ITERATE

100.0% PROCESSED 365 ITERATIONS

47 ANSWERS

SEARCH TIME: 00.00.01

L3 47 SEA SSS FUL L1

=> d cost

COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
CONNECT CHARGES	7.56	7.71
NETWORK CHARGES	1.26	1.32
SEARCH CHARGES	155.00	155.00
FULL ESTIMATED COST	163.82	164.03

IN FILE 'REGISTRY' AT 17:37:00 ON 05 FEB 2004

=> d stf

L3 ANSWER 1 OF 47 REGISTRY COPYRIGHT 2004 ACS on STN

ACNH-CH2-CH2-NH

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

=> d his

(FILE 'HOME' ENTERED AT 17:23:02 ON 05 FEB 2004)

FILE 'REGISTRY' ENTERED AT 17:23:32 ON 05 FEB 2004

L1 STRUCTURE UPLOADED

L2 1 S L1 SAM

L3 47 S L1 FULL

=> file caplus

COST IN U.S. DOLLARS SINCE FILE TOTAL

ENTRY SESSION

FULL ESTIMATED COST 166.79 167.00

FILE 'CAPLUS' ENTERED AT 17:39:55 ON 05 FEB 2004 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT. PLEASE SEE "HELP USAGETERMS" FOR DETAILS. COPYRIGHT (C) 2004 AMERICAN CHEMICAL SOCIETY (ACS)

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FILE COVERS 1907 - 5 Feb 2004 VOL 140 ISS 6 FILE LAST UPDATED: 4 Feb 2004 (20040204/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s 13

11 L3

=> d fbib abs hitstr total

L4 ANSWER 1 OF 11 CAPLUS COPYRIGHT 2004 ACS on STN

AN 2003:570644 CAPLUS

DN 139:133575

TI Preparation of bicyclic pyrimidinyl derivatives as adenosine receptor ligands grating clams
to look pat.

IN Castelhano, Arlindo L.; McKibben, Bryan

OSI Pharmaceuticals Inc., USA PA

SO U.S. Pat. Appl. Publ., 105 pp. CODEN: USXXCO

DTPatent

LA English

FAN.CNT 1

PATENT NO.	KIND	DATE

PΙ US 2003139427 **A1** 20030724

OS MARPAT 139:133575

GI

APPLICATION NO. DATE

US 2002-227378 20020823

US 2002-227378 20020823

 R^4 Ι

Title compds. I [Y = N, CR5 and X = N, CR6 wherein X, Y are both N or when

10/935753

AB

Y = CR5, X = N or when X = CR6, Y = N; R1-2 = H, alkoxy, aminoalkyl, etc; R3-4 = H, alkyl, aryl, alkylaryl] are prepared For instance, 3-amino-4-carbamoylpyrazole is acylated with benzoyl chloride (Pyridine, 50°, 5-6 h), cyclized to the corresponding pyrazolopyrimidine (water, K2CO3, 100°, 16 h), converted to the chloride (POCl3, 106°, 2 h) and used for reactions with various amines to give the example compds., e.g., II. II has Ki = 76.7 nM for the adenosine A1 receptor, Ki = 242.7 nM for A2a and Ki = 1480.5 nM for A2b. I are useful for the treatment of.

246855-42-5P 251946-07-3P 251946-08-4P
251946-37-9P 251946-38-0P 251946-39-1P

246855-42-5P 251946-07-3P 251946-08-4P 251946-37-9P 251946-38-0P 251946-39-1P 251946-40-4P 251946-41-5P 251946-45-9P 251946-46-0P 343632-20-2P 343632-31-5P 343632-32-6P 343632-37-1P 343632-38-2P 343632-39-3P 343632-40-6P 343632-41-7P 343632-43-9P 343632-44-0P 343632-45-1P

343632-46-2P 343969-97-1P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of bicyclic pyrazolo- imidazo- and triazolopyrimidinyl derivs. as adenosine receptor ligands)

RN 246855-42-5 CAPLUS

IT

CN

Acetamide, N-[2-[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]ethyl]- (9CI) (CA INDEX NAME)

 $AcNH-CH_2-CH_2-NH$

RN 251946-07-3 CAPLUS

CN Cyclopentanol, 3-[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]-, (1R,3R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 251946-08-4 CAPLUS

CN Cyclopentanol, 3-[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]-, (1R,3S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 251946-37-9 CAPLUS

CN Acetamide, N-[2-[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]-1-methylethyl]- (9CI) (CA INDEX NAME)

RN 251946-38-0 CAPLUS

CN Acetamide, N-[(1R)-2-[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]-1-methylethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 251946-39-1 CAPLUS

CN Acetamide, N-[(2R)-2-[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]propyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 251946-40-4 CAPLUS

CN Acetamide, N-[(1S)-2-[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]-1-methylethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 251946-41-5 CAPLUS

CN Acetamide, N-[(2S)-2-[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]propyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 251946-45-9 CAPLUS

CN Acetamide, N-[2-[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]-1,1-dimethylethyl]- (9CI) (CA INDEX NAME)

RN 251946-46-0 CAPLUS

CN Acetamide, N-[2-[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]propyl]- (9CI) (CA INDEX NAME)

RN 343632-20-2 CAPLUS

CN Acetamide, N-[2-[(2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]ethyl]-(9CI) (CA INDEX NAME)

RN 343632-31-5 CAPLUS

CN Acetamide, N-[1-[[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]methyl]-2-methylpropyl]- (9CI) (CA INDEX NAME)

RN 343632-32-6 CAPLUS

CN Urea, N'-[2-[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]ethyl]-N,N-diethyl- (9CI) (CA INDEX NAME)

RN 343632-33-7 CAPLUS

CN Ethanethioamide, N-[2-[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]ethyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & & H & Me \\ & & & & N & Me \\ & & & & \\ S & & & & \\ Me-C-NH-CH_2-CH_2-NH & & Me \\ \end{array}$$

RN 343632-35-9 CAPLUS

CN Urea, N-[3-[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]propyl]-N'-ethyl- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & & \\ & & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ &$$

RN 343632-36-0 CAPLUS

CN Glycine, 3-[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]cyclopentyl ester (9CI) (CA INDEX NAME)

RN 343632-37-1 CAPLUS

CN Cyclopentanol, 3-[(2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]- (9CI) (CA INDEX NAME)

RN 343632-38-2 CAPLUS

CN 1H-Pyrrole-2-carboxamide, N-[2-[(2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]ethyl]- (9CI) (CA INDEX NAME)

RN 343632-39-3 CAPLUS

CN 2-Imidazolidinone, 1-[2-[(2,6-diphenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]ethyl]- (9CI) (CA INDEX NAME)

RN 343632-40-6 CAPLUS

CN Butanamide, 2-[(2,6-diphenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]-3-methyl- (9CI) (CA INDEX NAME)

RN 343632-41-7 CAPLUS

CN Benzenepropanamide, α -[(2,6-diphenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]- (9CI) (CA INDEX NAME)

RN 343632-43-9 CAPLUS

CN 1H-Pyrrolo[2,3-d]pyrimidin-4-amine, 6-[(3-chlorophenoxy)methyl]-2-phenyl-N-[2-(1H-pyrrol-2-yl)ethyl]- (9CI) (CA INDEX NAME)

RN 343632-44-0 CAPLUS

CN Acetamide, N-[2-[[2-phenyl-6-[[(2S)-2-[(phenylamino)methyl]-1-pyrrolidinyl]methyl]-1H-pyrrolo[2,3-d]pyrimidin-4-yl]amino]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 343632-45-1 CAPLUS

CN Benzeneethanol, β -[[6-[(3-chlorophenoxy)methyl]-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl]amino]-, (β S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 343632-46-2 CAPLUS

CN 1-Piperidinecarboxamide, 2-[[[6-[(3-chlorophenoxy)methyl]-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl]amino]methyl]-N-methyl- (9CI) (CA INDEX NAME)

RN 343969-97-1 CAPLUS

CN 1,2-Cyclopentanediol, 4-[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]-, (1α , 2α , 4β)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

```
L4
        ANSWER 2 OF 11 CAPLUS COPYRIGHT 2004 ACS on STN
ΑN
        2003:511094 CAPLUS
        139:85365
DN
TI
        Preparation of pyrrolopyrimidine A2b selective antagonist compounds,
        method of synthesis and therapeutic use
IN
        Castelhano, Arlindo L.; Mckibben, Bryan; Steinig, Arno G.
PA
        Osi Pharmaceuticals, Inc., USA
        (PCT) Int. Appl., 223 pp.
SO
        CODEN: PIXXD2
DT
        Patent
LΑ
        English
FAN.CNT 1
        PATENT NO.
                                   KIND
                                            DATE
                                                                     APPLICATION NO.
                                                                                                DATE
ΡI
        WO 2003053361
                                     ΑŻ
                                             20030703
                                                                     WO 2002-US40890
                                                                                                20021220
        WO 2003053361
                                     Α3
                                             20031224
                    AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD,
                    RU, TJ, TM
              RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML,
                    MR, NE, SN, TD, TG
                                                                     US 2001-343443PP 20011220
        US 2003229067 .
                                             20031211
                                                                     ับร 2002-326005
                                    A1
                                                                                                20021220
                                                                     US 2001-343443PP 20011220
os
        CASREACT 139:85365; MARPAT 139:85365
GI
```

The subject invention provides pyrrolopyrimidines (shown as I; see below AB for variable definitions; e.g. N-[2-[6-[1-[2-(2chlorophenyl)ethyl]piperidin-4-yloxymethyl]-2-phenyl-7H-pyrrolo[2,3d]pyrimidin-4-ylamino]ethyl]acetamide (II)) or a specific enantiomer thereof, or a specific tautomer thereof, or a pharmaceutically acceptable salt thereof, and a method for treating a disease associated with the A2b adenosine receptor. For I: R1 is a (un)substituted alkyl (substituent = hydroxyl, dihydroxy, carboxyl, -C(O)NRaRb, -NRaC(O)NRaRb, -NRaC(O)NRaRb, or -NHC(O)Ra). R2 is H or a (un)substituted alkyl (substituent = hydroxyl, dihydroxyl, carboxyl, -C(O)NRaRb, -NRaC(O)NRaRb, -NRAC(O)NRAC(O)NRARb, -NRAC(O)NRAC(together form a substituted piperazine, substituted azetidine, or a pyrrolidine ring substituted with -(CH2)20H or -CH2C(O)OH. R3 is a (un) substituted Ph or a 5-6 membered heteroaryl ring, wherein the substituent is halogen, hydroxyl, cyano, (C1-C15) alkyl, (C1-C15) alkoxyl or -NRaRb; R4 is H or (un) substituted (C1-C15) alkyl; R5 is -(CH2) mOR6, -CHNOR7, -C(0)NR8R9, -(CH2)mC(0)OR10, -(CH2)kC(0)NR11R12; addnl. details are given in the claims. Radioligand binding assays yielded selectivities for the A2b receptor relative to the A1, A2a and A3 receptors for 9 examples of I, e.g. 26 times for II. About 26 example prepns. of I and intermediates and characterization data for hundreds of I and intermediates are included. For example, III can be prepared by reacting 4-chloro-2-phenyl-7H-pyrrolo[2,3-d]pyrimidine with PhSO2Cl and a reducing agent in the presence of solvent to produce 7-benzenesulfony1-4-chloro-2phenyl-7H-pyrrolo[2,3-d]pyrimidine, which was reacted with CO2 in the presence of LDA and a solvent to produce lithium 7-benzenesulfonyl-4chloro-2-phenyl-7H-pyrrolo[2,3-d]pyrimidine-6-carboxylate, which was reacted with AcNHCH2CH2NH2 in the presence of solvent to give 4-(2-acetylaminoethylamino)-7-benzenesulfonyl-2-phenyl-7H-pyrrolo[2,3d]pyrimidine-6-carboxylic acid, which was deprotected with a hydroxide base and subsequently condensed with amines. **343632-45-1P**, (S) -2 - [[6 - (3 - Chlorophenoxymethyl) - 2 + phenyl - 7H - (S) - 2 - [[6 - (3 - Chlorophenoxymethyl) - 2 + phenyl - 7H - (S) - 2 - [[6 - (3 - Chlorophenoxymethyl) - 2 + phenyl - 7H - (S) - 2 - [[6 - (3 - Chlorophenoxymethyl) - 2 + phenyl - 7H - (S) - 2 - [[6 - (3 - Chlorophenoxymethyl) - 2 + phenyl - 7H - (S) - 2 - [[6 - (3 - Chlorophenoxymethyl) - 2 + phenyl - 7H - (S) - 2 - [[6 - (3 - Chlorophenoxymethyl) - 2 + phenyl - 7H - (S) - 2 - [[6 - (3 - Chlorophenoxymethyl) - 2 + phenyl - 7H - (S) - 2 - [[6 - (3 - Chlorophenoxymethyl) - 2 + phenyl - 7H - (S) - 2 - [[6 - (3 - Chlorophenoxymethyl) - 2 + phenyl - 7H - (S) - 2 - [[6 - (3 - Chlorophenoxymethyl) - 2 + phenyl - 7H - (S) - 2 - [[6 - (3 - Chlorophenoxymethyl) - 2 + phenyl - 7H - (S) - 2 - [[6 - (3 - Chlorophenoxymethyl) - 2 + phenyl - 7H - (S) - 2 - [[6 - (3 - Chlorophenoxymethyl) - 2 + phenyl - 7H - (S) - 2 - [[6 - (3 - Chlorophenoxymethyl) - 2 + phenyl - 7H - (S) - 2 - [[6 - (3 - Chlorophenoxymethyl) - 2 + phenyl - 7H - (S) - 2 - [[6 - (3 - Chlorophenoxymethyl) - 2 + phenyl - 7H - (S) - 2 - [[6 - (3 - Chlorophenoxymethyl) - 2 + phenyl - 2 - [[6 - (3 - Chlorophenoxymethyl) - 2 + phenyl - 2 - [[6 - (3 - Chlorophenoxymethyl) - 2 + phenyl - 2 - [[6 - (3 - Chlorophenoxymethyl) - 2 + phenyl - 2 - [[6 - (3 - Chlorophenoxymethyl) - 2 + phenyl - 2 - [[6 - (3 - Chlorophenoxymethyl) - 2 + phenyl - 2 - [[6 - (3 - Chlorophenoxymethyl) - 2 + phenyl - 2 - [[6 - (3 - Chlorophenoxymethyl) - 2 + phenyl - 2 - [[6 - (3 - Chlorophenoxymethyl) - 2 + phenyl - 2 - [[6 - (3 - Chlorophenoxymethyl) - 2 - [6 - (3 - ChlorophenoxymIT pyrrolo[2,3-d]pyrimidin-4-yl]amino]-2-phenylethanol 343632-46-2P , 2-[[[6-(3-Chlorophenoxymethyl)-2-phenyl-7H-pyrrolo[2,3-d]pyrimidin-4yl]amino]methyl]piperidine-1-carboxylic acid methylamide 343632-81-5P, (R)-2-[[6-(3-Chlorophenoxymethyl)-2-phenyl-7Hpyrrolo[2,3-d]pyrimidin-4-yl]amino]-2-phenylethanol 553631-99-5P , N-[2-[[6-(3-Chlorophenoxymethyl)-2-phenyl-7H-pyrrolo[2,3-d]pyrimidin-4yl]amino]ethyl]acetamide 553632-26-1P, N-[2-[[6-(3-Chlorophenoxymethyl) -5-[(dimethylamino)methyl] -2-phenyl-7H-pyrrolo[2,3d]pyrimidin-4-yl]amino]ethyl]acetamide 553634-62-1P, N-[2-[(2-Phenyl-6-((S)-2-[(phenylamino)methyl]pyrrolidine-1-carbonyl)-7H-

pyrrolo[2,3-d]pyrimidin-4-yl]amino]ethyl]acetamide RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses) (drug candidate; preparation of pyrrolopyrimidine A2b selective antagonist compds., method of synthesis and therapeutic use) RN343632-45-1 CAPLUS CN Benzeneethanol, β -[[6-[(3-chlorophenoxy)methyl]-2-phenyl-1Hpyrrolo[2,3-d]pyrimidin-4-yl]amino]-, (βS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 343632 46-2 CAPLUS

1-Piperidinecarboxamide, 2-[[[6-[(3-chlorophenoxy)methyl]-2-phenyl-1H-CNpyrrolo[2,3-d]pyrimidin-4-xl]amino]methyl]-N-methyl- (9CI) (CA INDEX NAME)

343632-81-5 CAPLUS RN

Benzeneethanol, β -[[6-[(3-chlorophenoxy)methyl]-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl]amino], (β R) - (9CI) (CA INDEX NAME) CN

Absolute stereochemistry.

RN 553631-99-5 CAPLUS

CN Acetamide, N-[2-[[6-[(3-chlorophenoxy)methyl]-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl-]amino]ethyl]- (9CI) (CA INDEX NAME)

Ph N
$$H$$
 CH_2-O $C1$
ACNH- CH_2-CH_2-NH

RN 553632-26-1 CAPLUS

CN Acetamide, N-[2-[[6-[(3-chlorophenoxy)methyl]-5-[(dimethylamino)methyl]-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl]amino]ethyl]- (9CI) (CA INDEX NAME)

 ${\tt AcNH-CH_2-CH_2-NH}$

RN 553634-62-1 CAPLUS

CN Acetamide, N-[2-[[2-phenyl-6-[[(2S)-2-[(phenylamino)methyl]-1-pyrrolidinyl]carbonyl]-1H-pyrrolo[2,3-d]pyrimidin-4-yl]amino]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

```
L4
       ANSWER 3 OF 11
                               CAPLUS
                                           COPYRIGHT 2004 ACS on STN
AN
       2003:454286 CAPLUS
DN
       139:36534
TI
       Preparation/of arylpyrrolopyrimidines as adenosine A1 and A3 receptor
       inhibitors
IN
       Castelhano/ Arlindo L.; McKibben, Bryan; Werner, Douglas S.; Witter, David
       OSI Pharmaceuticals, Inc., USA
PA
       PCT) Int. Appl., 170 pp.
SO
       CODEN: PIXXD2
DT
       Patent
       English
LΑ
FAN.CNT 1
       PATENT NO.
                                KIND
                                         DATE
                                                                APPLICATION NO.
                                 _ _ _ _
PΙ
       WO 2003048120
                                  Α2
                                          20030612
                                                                WO 2002-US38055
                                                                                         20021127
       WO 2003048120
                                  Α3
                                          20030904
             W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,
                   CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH,
                   PL, PT, RO, RU, SC, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
             RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR,
                   NE, SN, TD, TG
                                                                US 2001-335273PP 20011130
                                                                US 2001-337274PP 20011130
os
       MARPAT 139:36534
GΙ
                 HN(CH<sub>2</sub>)mCH<sub>2</sub>R<sup>2</sup>
                                        Ι
```

AB Arylpyrrolopyrimidines I [m = 0-3; R = halogen, alkyl, alkoxy, OH, NH2, alkylamino; R1 = H, (un)substituted alkyl, aryl, aralkyl; R2 = (un)substituted imidazole, pyrazole, attached through C] which

```
specifically inhibit the adenosine A1 and A3 receptors were prepared Thus,
     4-chloro-2-phenyl-7H-pyrrolo[2,3-d]pyrimidine was treated with histamine
     to give the 4-[2-(1H-imidazol-2-yl)ethyl]amino analog which had A3
     inhibiting activity ≥10 times greater than that of reference compds.
     343632-31-5P 343632-32-6P 343632-33-7P
     343632-35-9P 343632-36-0P 343632-37-1P
     343632-38-2P 343632+39-3P 343632-43-9P
     343632-44-0P 343632-45-1P 343632-46-2P
     541504-10-3P 541504-12-5P
     RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological
     study); PREP (Preparation); USES (Uses)
        (preparation of arylpyrrolopyrimidines as adenosine A1 and A3 receptor
        inhibitors)
RN
     343632-31-5 CAPLUS
CN
     Acetamide, N-[1-[[5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-
     yl)amino]methyl]-2[methylpropyl]- (9CI) (CA INDEX NAME)
        Ph
                        Me
     NHAc
                       Me
i-Pr-CH-CH_2-NH
RN
     343632-32-6 CAPLUS
     Urea, N'-[2-[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-
CN
     yl)amino]ethyl]-N, N diethyl- (9CI) (CA INDEX NAME)
                                Me
                               Me
Et_2N-C-NH-CH_2-CH_2-NH
RN
     343632-33-7 CAPLUS
     Ethanethioamide, N-[2-[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-
CN
     yl)amino]ethyl]- (9CI) (CA INDEX NAME)
                              Мe
                            Me
Me-C-NH-CH_2-CH_2-NH
RN
     343632-35-9 CAPLUS
CN
     Urea, N-[3-[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d])pyrimidin-4-
     yl)amino]propyl]-N'-ethyl- (9CI) (CA INDEX NAME)
```

```
c = 0
         NH
         CH<sub>2</sub>
         CH<sub>2</sub>
        ŅΗ
Ph
       343632\\39-3 CAPLUS
RN
       2-Imidazolidinone, 1-[2-[(2,6-diphenyl-1H-pyrrolo[2,3-d]pyrimidin-4-
CN
       yl)amino)ethyl] - (9CI) (CA INDEX NAME)
        CH<sub>2</sub>
        CH<sub>2</sub>
        NH
                      Ph
Ph
RN
      343632-43-9 CAPLUS
      1H-Pyrrolo[2,3-d]pyrimidin-4-amine, 6-[(3-chlorophenoxy)methyl]-2-phenyl-N-[2-(1H-pyrrol-2-yl)ethyl]- (9CL) (CA INDEX NAME)
CN
```

RN 343632-44-0 CAPLUS

CN Acetamide, N-[2-[[2-phenyl-6-[[(2S)-2-[(phenylamino)methyl]-1-pyrrolidinyl]methyl]-1H-pyrrolo[2,3-d]pyrimidin-4-yl]amino]ethyl]- (9CI) (CA:INDEX NAME)

Absolute stereochemistry.

RN 343632-45-1 CAPLUS

CN Benzeneethanol, β -[[6-[(3-chlorophenoxy)methyl]-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl]amino]-, (β S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 343632-46-2 CAPLUS

CN 1-Piperidinecarboxamide, 2-[[[6-[(3-chlprophenoxy)methyl]-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl]amino]methyl]-N-methyl-(9CI) (CA INDEX NAME)

CN Butanamide 2-[(2,6-diphenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]-3-methyl-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 541504-12-5 CAPLUS

CN Benzenepropanamide, α -[(2,6-diphenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]-, (α S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L4 ANSWER 4 OF 11 CAPLUS COPYRIGHT 2004 ACS on STN

AN 2003:300617 CAPLUS

DN 138:321287

TI Preparation of deazapurines as adenosine A3 receptor antagonists.

IN Castelhano, Arlindo L.; McKibben, Bryan; Witter, David J.

```
OSI Pharmaceuticals, Inc., USA
     U.S. Pat. Appl. Publ., 77 pp.
SO
     CODEN: USXXCO
DT
     Patent
LA
     English
FAN.CNT 1
     PATENT NO.
                       KIND
                             DATE
                                              APPLICATION NO.
                                                              DATE
PΙ
     US 2003073708
                        A1
                              20030417
                                              US 2001-6405
                                                                20011130
     US -66738021
                        B2
                              20040106
                                              US 2000-250748PP 20001201
os
     MARPAT 138:321287
GΙ
      NR1R2
                 R5
                     Ι
AΒ
     Title comp\(ds. [I; R1, R2 = H, (substituted) alkyl, aryl, aralkyl; R1R2 =
     atoms to form (substituted) heterocyclyl; R3 = (substituted) alkyl, aryl,
     aralkyl; R4 = H, (substituted) alkyl, aryl, aralkyl; R5, R6 = H, halo,
     (substituted) alkyl, aryl, alkylaryl; R4R5 or R5R6 = (substituted) heterocyclyl, carbocyclyl], were prepared Thus, 2-phenyl-7H-pyrrolo[2,3-
     d]pyrimidin-4-ylamine and histamine were heated at 120° in Me2SO
     for 6.5 h to give 43% [2-(3H-imidazol-4-yl)ethyl] [2-phenyl-7H-pyrrolo[2,3-
     d]pyrimidin-4-yl]amine. The latter had 10 times the A3 receptor binding
     affinity of a reference compound
IT
     246855-42-5P 251946-07-3P 251946-08-4P
     251946-09-5P 251946-37-9P\251946-38-0P
     251946-39-1P 251946-40-4P 251946-41-5P
     251946-45-9P 251946-46-0P 251946-55-1P
     343632-31-5P 343632-32-6P 343632-35-9P
     343632-37-1P 343632-38-2P 343632-39-3P
     343632-40-6P 343632-41-7P 343632-43-9P
     343632-44-0P 343632-45-1P 343632-46-2P
     500736-03-8P
     RL: PAC (Pharmacological activity); SPN\(Synthetic preparation); THU
     (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
     (Uses)
         (preparation of deazapurines as adenosine A3 receptor antagonists)
RN
     246855-42-5 CAPLUS
     Acetamide, N-[2-[(5,6-dimethyl-2-phenyl-1H\pyrrolo[2,3-d]pyrimidin-4-
CN
     yl)amino]ethyl]- (9CI) (CA INDEX NAME)
                         Me
AcNH-CH2-CH2-NH
```

RN 251946-07-3 CAPLUS

CN Cyclopentanol, 3-[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]-, (1R,3R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 251946-08-4 CXPLUS

CN Cyclopentanol 3-[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]-, (1R,3S)-rel- (9CI) (CA INDEX NAME)

Relative stereoghemistry.

RN 251946-09-5 CAPLUS

CN 1,2-Cyclopentanediol, 4-[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]-, stereoisomer (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 251946-37-9 CAPLUS

CN Acetamide, N-[2-[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]-1-methylethyl]- (9CI) (CA INDEX NAME)

RN 251946-38-0 CAPLUS

CN Acetamide, N-[(1R)-2-[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]-1-methylethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 251946-39-1 CAPLUS

CN Acetamide, N-[(2R)-2-[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]propyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 251946-40-4 CAPLUS

CN Acetamide, N-[(1S)-2-[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]-1-methylethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN251946-41-5 CAPLUS Acetamide, N-[(2S)-2-[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-CN(ĆA INDEX NAME) yl)amino]propyl] - (9CI) Absolute stereochemistry. Me Me AcNH Me RN 251946-45-9 CAPLUS CN Acetamide, N-[2-[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4yl)amino]-1,1-dimethylethyl]- (9CI) (CA INDEX NAME) Me AcNH Me -сн₂ — ин Me RN 251946-46-0 CAPLUS CN Acetamide, N-[2-[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4yl)amino]propyl]- (9GĮ) (CA INDEX NAME) Me Me AcNH-CH2-CH-NH Me RN251946-55-1 CAPLUS CNAcetamide, N-[1-[[(5,6-dimethyll-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4yl)amino]methyl]propyl] - (9CI) (CA INDEX NAME)

RN 343632-31-5 CAPLUS

CN Acetamide, N-[1-[[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]methyl]-2-methylpropyl]- (9CI) (CA INDEX NAME)

RN 343632-32-6 CAPLUS

CN Urea, N'-[2-[\(\frac{1}{5}\),6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]ethyl]-N,N-diethyl- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & & \\ & & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & \\ & & & \\ & &$$

RN 343632-35-9 CAPLUS

CN Urea, N-[3-[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]propyl]-N'-ethyl- (9CI) (CA INDEX NAME)

RN 343632-37-1 CAPLUS

CN Cyclopentanol, 3-[(2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]- (9CI) (CA INDEX NAME)

RN 343632-38-2 CAPLUS

CN 1H-Pyrrole-2-carboxamide, N-[2-[(2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]ethyl]- (9CI) (CA INDEX NAME)

RN 343632-39-3 CAPLUS

CN 2-Imidazolidinone, 1-[2-[(2,6-diphenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]ethyl]- (9CI) (CA INDEX NAME)

```
RN
      343632-40-6 CAPLUS
CN
      Butanamide, 2-[(2,6-diphenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]-3-
      methyl- (9CI) (CA INDEX NAME)
 H<sub>2</sub>N-
i-Pr-CH-NH
    Ph
RN
      343632-41-7 CAPLUS
CN
      Benzenepropanamide, \alpha - (2,6-diphenyl-1H-pyrrolo[2,3-d]pyrimidin-4-
                           (CA INDEX NAME)
      yl)amino]- (9CI)
        CH2-Ph
H2N-C-CH-NH
                         Ph
RN
      343632-43-9 CAPLUS
      1H-Pyrrolo[2,3\d]pyrimidin-4-amine, 6-[(3-chlorophenoxy)methyl]-2-phenyl-N-
CN
      [2-(1H-pyrrol-2\yl)ethyl]- (9CI) (CA INDEX NAME)
       CH<sub>2</sub>
       CH<sub>2</sub>
       NH
Ph
RN
      343632-44-0 CAPLUS
      Acetamide, N-[2-[[2-phenyl-6-[[(2S)-2-[(phenylamino)methyl]-1-pyrrolidinyl]methyl]-1H-pyrrolo[2,3-d]pyrimidin-4-yl]amino]ethyl]- (9CI)
CN
      (CA INDEX NAME)
Absolute stereochemistry.
```

CM

1

CRN 251946-51-7 CMF C21 H25 N5 O2

Relative stereochemistry.

$$H_2N$$
 O
 S
 R
 NH
 Me
 NH
 Me
 NH

CM 2

CRN 76-05-1 CMF C2 H F3 O2

L4 ANSWER 5 OF 11 CAPLUS COPYRIGHT 2004 ACS on STN

AN 2003:174478 CAPLUS

DN 138:221598

TI Preparation of pyrrolo[2,3-d]pyrimidinamines as selective adenosine A1 receptor inhibitors for treatment of asthma, COPD, and other conditions

IN Castelhano, Arlindo L.; McKibben, Bryan; Witter, David J.

PA OSI Pharmaceuticals, Inc., USA

SO U.S. Pat. Appl. Publ., /79 pp.

CODEN: USXXCO

DT Patent

LA English

FAN.CNT 1

PATENT NO. KIND DATE

PI US 2003:045536 A1 20030306 US 6680324 B2 20040120

OS MARPAT 138:221598

GΙ

APPLICATION NO. DATE

US 2001-280 20011130

US 2000-250895PP 20001201

$$R^{1}$$
 R^{2}
 R^{6}
 R^{3}
 R^{4}
 R^{4}
 R^{5}
 R^{1}
 R^{2}
 R^{6}
 R^{7}
 R^{7}
 R^{7}
 R^{7}
 R^{7}
 R^{1}
 R^{2}
 R^{5}
 R^{7}
 R^{7

AΒ Title diazapurinamines I [wherein R1, R2, and R4 = independently H or (un) substituted alkyl(aryl) or aryl; or NR1R2 = (un) substituted heterocyclyl; R3 (= (un) substituted alkyl(aryl), aryl, CO2H, carboxy esters, or carboxamides; or C2R3R4 or C2R5R6 = (un) substituted carbocyclyl or heterocyclyl; R5 and R6 = independently H, halo, or (un) substituted alkyl(aryl) or aryl; and pharmaceutically acceptable salts and prodrugs thereof] were prepared as adenosine A1 specific inhibitors. For example, 4-chloro-5-methyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidine was protected with di-t-Bu dicarbonate (80%), brominated (84%), coupled with anhydrous Me glycolate (99%), coupled with L-prolinamide (92%), and deprotected (93%) to give II. The latter exhibited adenosine Al receptor binding equal to or surpassing that of reference compds. and is expected to have better water solubility (cLogP = 1.5) than reference compds. (cLogP = 3.8). Efficacy and structure activity profiles of diazapurines of the invention are also disclosed. Thus, I are useful for the treatment of asthma, chronic obstructive pulmonary disease (COPD), allergic rhinitis, upper respiratory disorder, and congestive heart failure (no data).

IT 251946-08-4P

RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOI (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

(Al receptor inhibitor; preparation of pyrrolopyrimidinamines adenosine Al receptor inhibitors from aminocyanopyrroles for treatment of asthma, COPD, and other conditions)

RN 251946-08-4 CAPLUS

Cyclopentanol, 3-[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]-, (1R,3S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

CN

```
Me
IT
     246855-42-5P, 4-[(2/Acetylaminoethyl)amino]-5,6-dimethyl-2-phenyl-
     7H-pyrrolo[2,3-d]pyrimidine 251946-07-3P, 4-[(3-trans-
     Hydroxycyclopentyl∦amino]-5,6-dimethyl-2-phenyl-7H-pyrrolo[2,3-
     d]pyrimidine 251946-37-9P, 4-[(2-Acetylaminopropyl)amino]-5,6-
     dimethyl-2-phenyl\frac{1}{i}7H-pyrrolo[2,3-d]pyrimidine 251946-38-0p,
     (R)-4-[(2-Acetylaminopropyl)amino]-5,6-dimethyl-2-phenyl-7H-pyrrolo[2,3-
     d]pyrimidine 251946-39-1P, (R)-4-[(1-Methyl-2-
     acetylaminoethyl)amino]-5,6-dimethyl-2-phenyl-7H-pyrrolo[2,3-d]pyrimidine
     251946-40-4P, (S)-4-[(2-Acetylaminopropyl)amino]-5,6-dimethyl-2-
     phenyl-7H-pyrrolo[2,3-d]pyrimidine 251946-41-5P,
     (S)-4-[(1-Methyl-2-acetylaminoethyl)amino]-5,6-dimethyl-2-phenyl-7H-
     pyrrolo[2,3-d]pyrimidihe 251946-45-9P, 4-[(2-Methyl-2-
     acetylaminopropyl)aminoj\z5,6-dimethyl-2-phenyl-7H-pyrrolo[2,3-d]pyrimidine
     251946-46-0P, 4-[(1-Methyl-2-acetylaminoethyl)amino]-5,6-dimethyl-
     4-[(2-Acetamidobutyl)amino]-\$,6-dimethyl-2-phenyl-7H-pyrrolo[2,3-
     d]pyrimidine 343632-20-2P 343969-97-1P
     500736-03-8P
     RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
     (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
     (Uses)
        (Al receptor inhibitor; preparation of pyrrolopyrimidinamines adenosine A1
        receptor inhibitors from aminocyanopyrroles for treatment of asthma,
        COPD, and other conditions)
RN
     246855-42-5 CAPLUS
CN
     Acetamide, N-[2-[(5,6-dimethyl-2/phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-
     yl)amino]ethyl]- (9CI) (CA INDEX NAME)
                         Me
                        Me
ACNH-CH2-CH2-NH
RN
    251946-07-3 CAPLUS
    Cyclopentanol, 3-[(5,6-di/methyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-
CN
    yl)amino]-, (1R,3R)-rel-/(9CI) (CA INDEX NAME)
Relative stereochemistry.
```

10/035753

Acetamide, $N-\sqrt{2-[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-pyrrolo[2,3-d]pyrrolo[2,$ yl)amino]-1-methylethyl]- (9CI) (CA INDEX NAME)

251946-38-0 CAPLUS RN

CN Acetamide, N-[(1R)-2-[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4yl)amino]-1-methylethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 251946-39-1 | CAPLUS

CN Acetamide, N-[(2R)-2-[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4yl)amino]propyl] - (9CI) (CA INDEX NAME)

Absolute stereochemistry.

```
RN
     251946-40-4 CAPLUS
     Acetamide, N-[(1S)-2-[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-
CN
     yl)amino]-1-methylethyl]- (9CI) (CA INDEX NAME)
Absolute stereochemistry.
                      Me
 AcNH
                      Мe
Me
RN
     251946-41-5 CAPLÚS
     Acetamide, N-[(25)-2-[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-
CN
     yl)amino]propyl] (9CI) (CA INDEX NAME)
Absolute stereochemistry.
                        Me
AcNH
        Me
RN
     251946-45-9 CAPLUS
     Acetamide, N-[2-[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-
CN
     yl)amino]-1,1-dimethylethyl]- (9CI) (CA INDEX NAME)
                     Me
 AcNH
                    Мe
      -сн<sub>2</sub>-ин
  Me
RN
     251946-46-0 CAPLUS
     Acetamide, N-[2-[(5,6/dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-
CN
     yl)amino]propyl] - (901) (CA INDEX NAME)
```

RN 251946-55-1 CAPLUS

CN Acetamide, N-[1-[[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]methyl]propyl]- (9CI) (CA INDEX NAME)

RN 343632-20-2 CAPLUS

CN Acetamide, N-[2-[(2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]ethyl]-(9CI) (CA INDEX NAME)

RN 343969-97-1 CAPLUS

CN 1,2-Cyclopentanediol, 4-[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]-, $(1\alpha,2\alpha,4\beta)$ - (9Cl) (CA INDEX NAME)

Relative stereochemistry.

RN 500736-03-8 CAPLUS

CN Glycine, (1R,3S)-3-[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]cyclopentyl ester, rel-, trifluoroacetate (9CI) (CA INDEX NAME)

```
CM
          251946-51-47
     CRN
     CMF
          C21 H25/N5 O2
Relative stereochemistry.
                         NH
                               Мe
                                      Me
                                   NH
                  Ph
     CM
           2
     CRN
          76-05-1
          C2 H F3 O2
     CMF
  с-со2н
  F
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COPYRIGHT 2004 ACS on STN
L4
          ANSWER 6 OF 11 CAPLUS
          2002:555495 .CAPLUS
AN
          137:109485
DN
          Preparation of pyrrolopy imidinylprolineamides and analogs as adenosine
TI
          receptor antagonists
          Castelhano, Arlindo L. / McKibben, Bryan; Witter, David J.
IN
          Osi Pharmaceuticals, Inc., USA
PA
          PCT Int. Appl., 320 pp
so
         CODEN: PIXXD2
DT
          Patent
         English
LΑ
FAN.CNT 3
          PATENT NO.
                                            KIND
                                                        DATE
                                                                                       APPLICATION NO.
                                                                                                                          DATE
PI
          WO 2002057267
                                              A1
                                                         20020725
                                                                                       WO 2001-US45280
                                                                                                                          20011130
                 W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

US 1999-169037PP 19991202
                                                                                       ปร 2000-728316 A 20001201
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US 2000-728616 A 20001201
                                            US 2000-728607 A 20001204
     US 2002058667
                       A1
                             20020516
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     251946-40-4P 251946-41-5P 251946/45-9P
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        (preparation of pyrrolopyrimidinylprolineamides and analogs as adenosine
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RN
     246855-42-5 CAPLUS
     Acetamide, N-[2-[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-
CN
     yl)amino]ethyl]- (9CI)
                             (ÇA INDEX NAME)
10/035753
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RN 251946-07-3 CAPLUS

CN Cyclopentanol, 3-[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]-, (1R,3R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry

RN 251946-08-4 CAPLUS

CN Cyclopentanol 3-[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]-, (iR,3S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 251946-37-9 CAPIUS

CN Acetamide, N-[2-[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]-1-methylethyl]- (9CI) (CA INDEX NAME)

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      251946-38-0 CAPLUS
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      Acetamide, N-[(1R)-2-[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-
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                                          (CA/INDEX NAME)
Absolute stereochemistry.
                        Me
  AcNH
                       Me
Me
      251946-39-1 CAPLUS
RN
      Acetamide, N-[\sqrt{2}R)-2-[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-
CN
      yl)amino]propyĺ]- (9CI) (CA INDEX NAME)
Absolute stereochemistry.
                          Me
A¢NH
        Me
RN
      251946-40-4 CAPLÙS
     Acetamide, N-[(1S)^{1}2-[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]-1-methylethyl]- (9CI) (CA INDEX NAME)
CN
Absolute stereochemistry
                  Н
   Ph
                        Me
 AcNH
                       Мe
RN
     251946-41-5 CAPLUS
     Acetamide, N-[(2S) \frac{1}{2}-[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-
CN
                          (9CI)
     yl)amino]propyl]-
                                 (CA INDEX NAME)
Absolute stereochemistry.
10/035753
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         CH<sub>2</sub>
         NH
RN
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         CH<sub>2</sub>
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       Butanamide, 2-[(2,6-diphenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]-3-methyl- (9CI) (CA INDEX NAME)
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10/035753
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CN
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     yl)amino] - (9CI) (CA INDEX NAME)
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     Acetamide, N-[2-[[2-phenyl-6-[[(2S)-2-[(phenylamino)methyl]-1-
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     pyrrolidinyl]methyl]-1H-pyrrolo[2,3-d]pyrimidin-4-yl]amino]ethyl]- (9CI)
     (CA INDEX NAME)
Absolute stereochemistry.
                          PhNH
AcNH
RN
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CN
     Benzeneethanol, \beta-[[6-[(3-chlorophenoxy)methyl]-2-phenyl-1H-
     pyrrolo[2,3-d]pyrimidin-4-yl]amino]-, (βS)- (9CI) (CA INDEX NAME)
Absolute stereochemistry.
10/035753
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RN 343632-46-2 CAPLUS

CN 1-Piperidinecarboxamide, 2-[[[6-[(3-chlorophenoxy)methyl]-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl]amino]methyl]-N-methyl- (9CI) (CA INDEX NAME)

RN 343969-97-1 CAPLUS

CN 1,2-Cyclopentanediol, 4-[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]-, $\langle 1\alpha, 2\alpha, 4\beta \rangle$ - (9CI) (CA INDEX NAME)

Relative stereochemistry.

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THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

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Pyrrolopyrimidines I $[R = \frac{1}{3} - hydroxycyclopentylamino ethylamino$ AB carbonylamino Pr, N, N-diethylamino carbonylamino Et, thioacetamido Et, 3-amino acetyloxy cyclopentyl, 3-hydroxycyclopentyl, 2-pyrrolyl carbonyl aminoethyl, 2-imidazolinone Et, 1-aminocarbonyl-2-methylpropyl, 1-aminocarbonyl-2-Ph Et, 3-hydroxyazetidino, 2-imidazoleethyl, acetamidoethyl, 1-(R)-phenyl-2-hydroxyethyl, N-methylaminocarbonyl pyridyl-2-methyl; R1 = H; RRNN = 3-hydroxypyrrolidino, 3-methyloxy carbonylmethyl pyrrolidino, 3-aminocarbonylmethyl pyrrolidino, 3-hydroxymethyl piperidino; R3, R4 = H, (un) substituted alkyl, aryl] are prepared as selective inhibitors of adenosine receptors, particularly the adenosine A3 receptor, for the treatment of diseases such as asthma, diarrhea, chronic obstructive pulmonary disease, allergic rhinitis, or for the treatment of eye damage caused either by disease or injury. Human adenosine receptors are transformed into yeast; the modified yeast are used to assay the invention compds. I for their adenosine receptor binding and selectivities. E.g., 1-(1-phenylethyl)-2-amino-3-cyano-4,5dimethylpyrrole is acylated with PhCOCl to give the benzamide which undergoes cyclocondensation with concentrated H2SO4 in MeOH to give a pyrrolopyrimidinone; removal of the phenethyl group with polyphosphoric acid and chlorination of the pyrrolopyrimidinone with POCl3 gives the intermediate chloropyrrolopyrimidine II. E.g., addition of amines such as trans-3-amino-1-cyclopentanol to II in DMSO gives aminopyrrolopyrimidines such as III. III has a Ki for the adenosine Al receptor of 29 nM and a Ki for the adenosine A3 receptor of 3.1\nM while binding to the adenosine A2a and A2b receptors with Ki values of 191 nM and 1143 nM, resp. Formulations of these compds. are claimed (no data). Methods for the preparation of I from the acylation of aminopyrroles with acyl chlorides followed by cyclocondensation and deprotection, chlorination, and substitution of the chlorine atom with an amine are claimed.

TT 246855-42-5P 246855-48-1P 251946-07-3P 251946-08-4P 251946-37-9P 251946-38-0P 251946-39-1P 251946-40-4P 251946-41-5P 251946-45-9P 251946-46-0P 251946-52-8P 343632-31-5P 343632-32-6P 343632-37-1P 343632-38-2P 343632-39-3P 343632-40-6P 343632-41-7P 343632-43-9P 343632-44-0P 343632-45-1P 343632-46-2P 343632-77-9P 343632-78-0P 343632-79-1P 343632-80-4P

343632-81-5P 343632-82-6P 343632-83-7P 343633-16-9P 343969-97-1P 443118-58-9P RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses) (invention compound; preparation of pyrrolo[2,3-d]pyrimidines as selective inhibitors of the adenosine A3 receptor for the treatment of diseases such as diarrhea, allergic rhinitis, and eye damage resulting from injuries or disease) RN246855-42-5 CAPLUS Acetamide, N-[2-[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-CNyl)amino]ethyl]- (9Cl) (CA INDEX NAME) Me ACNH-CH2-CH2-NH RN246855-48-1 CAPLUS 2-Imidazolidinone, 1-[2-[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]ethyl]- (9CI) (CA INDEX NAME) CNCH₂ CH₂ Me NH Me NH Ph RN251946-07-3 CAPLUS CNCyclopentanol, 3-[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4yl)amino]-, (1R,3R)-rel- (9CI) (CA INDEX NAME) Relative stereochemistry.

RN 251946-08-4 CAPLUS

CN Cyclopentanol, 3-[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]-, (1R,3S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 251946-37-9 CAPLUS

CN Acetamide, N-[2-[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]-1-methylethyl]- (9CI) (CA INDEX NAME)

RN 251946-38-0 CAPLUS

CN Acetamide, N-[(1R)-2-[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]-1-methylethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 251946-39-1 CAPLUS

CN Acetamide, N-[(2R)-2-[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]propyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 251946-40-4 CAPLUS

CN Acetamide, N-[(1S)-2-[(5/6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]-1-methylethyl]/- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 251946-41-5 CAPLUS

CN Acetamide, N-[/(2S)-2-[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]propyl]- (9CI) (CA INDEX NAME)

Absolute stereochémistry.

RN 251946-45-9 CAPLUS

CN Acetamide, N-[2-[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]-1,1-dimethylethyl]- (9CI) (CA INDEX NAME)

RN 251946-46-0 CAPLUS

CN Acetamide, N-[2-[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]propyl]- (9CI) (CA INDEX NAME)

ACNH-CH2-CH-NH

RN 251946-52-8 CAPLUS

CN Glycine, (1R,3S)-3-[(5/6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]cyclopentyl ester, rel-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 251946-51-7 CMF C21 H25 N5 O2

Relative stereochemistry.

```
CO2H
RN
       343632-31-5 CAPLUS
      Acetamide, N-[1-[[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]methyl]-2-methylpropyl]- (9CI) (CA INDEX NAME)
          Ph.
                                Me
       NHAc
i-Pr-CH-CH2-NH
       343632-32-6 CAPLUS
RN
      Urea, N'-[2-[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]ethyl]-N,N-diethyl, (9CI) (CA INDEX NAME)
CN
                                          Me
                                         Me
Et_2N-C-NH-CH_2-CH_2-NH
RN
      343632-33-7 CAPLUS
      Ethanethioamide, N-[2-[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]ethyl]- /(9CI) (CA INDEX NAME)
CN
                                Н
                                       Me
                                      Me
Me-C-NH-CH_2-CH_2-NH
RN
      343632-35-9 CAPLUS
      Urea, N-[3/[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-
CN
      yl)amino]propyl]-N'-ethyl- (9CI) (CA INDEX NAME)
                                Η
                                       Me
                                      Me
EtNH-C-NH-\frac{1}{2} (CH<sub>2</sub>)<sub>3</sub>-NH
10/035753
```

RN 343632-36-0 CAPLUS

CN Glycine, 3-[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]cyclopentyl ester (9CI) (CA INDEX NAME)

$$H_2N-CH_2-C-O$$

NH Me

NH Me

Ph

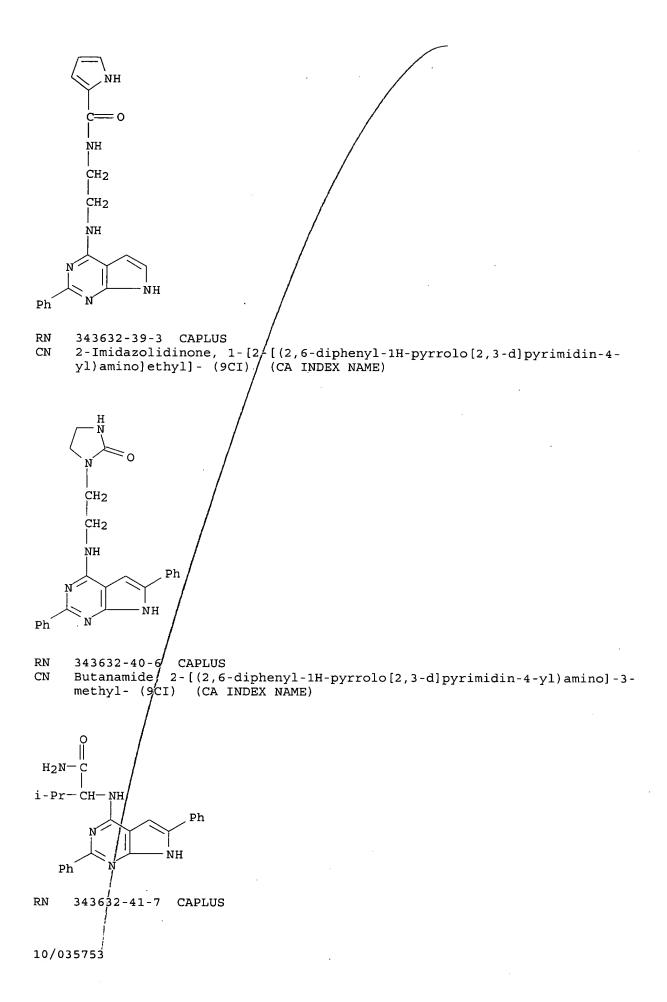
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RN 343632-37-1 CAPLUS

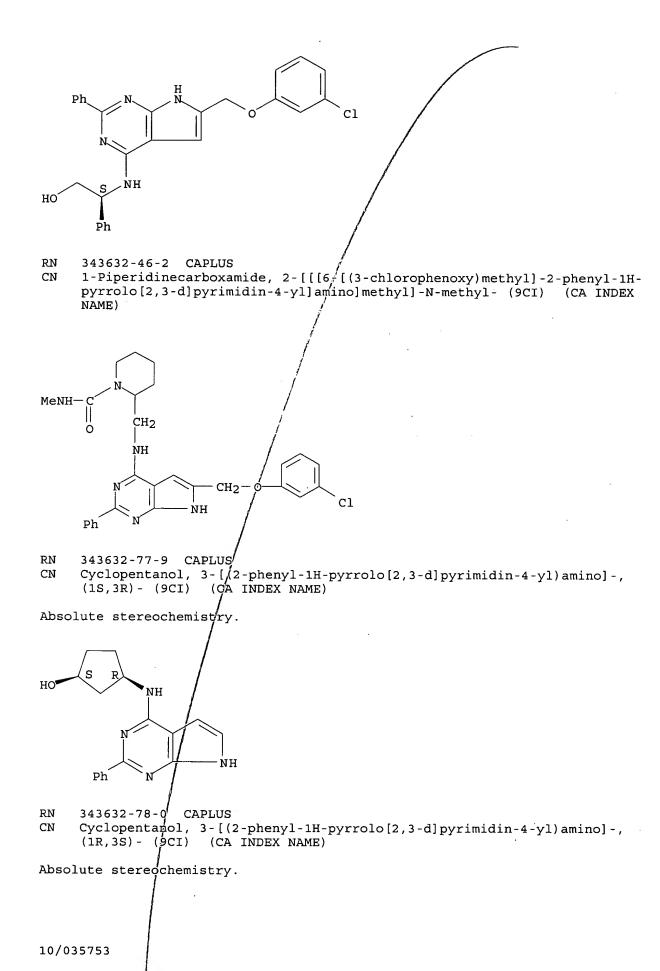
CN Cyclopentanol, 3-[(2-phenyl-AH-pyrrolo[2,3-d]pyrimidin-4-yl)amino]- (9CI) (CA INDEX NAME)

RN 343632-38-2 CAPLUS

CN 1H-Pyrrole-2-carboxamide, N-[2-[(2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]ethyl]- (9CI) (CA INDEX NAME)



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CN
      Benzenepropanamide, \alpha-[(2,6-diphenyl-1H-pyrrolo[2,3-d]pyrimidin-4-
      yl)amino] - (9CI) (CA INDEX NAME)
        CH2-Ph
H2N-C-CH-NH
     Ph
RN
      343632-43-9 CAPLUS
CN
      1H-Pyrrolo[2,3-d]pyrimidin-4-amine, 6-[(3-chlorophenoxy)methyl]-2-phenyl-N-
      [2-(1H-pyrrol-2-yl)ethyl]- (9C/1) (CA INDEX NAME)
       CH<sub>2</sub>
       CH<sub>2</sub>
       NH
                                     Cl
Ph
RN
      343632-44-0 CAPLUS
     Acetamide, N-[2-[[2/-phenyl-6-[[(2S)-2-[(phenylamino)methyl]-1-pyrrolidinyl]methyl]-1H-pyrrolo[2,3-d]pyrimidin-4-yl]amino]ethyl]- (9CI)
CN
      (CA INDEX NAME)
Absolute stereochemistry.
                            PhNH
AcNH
RN
     343632-45-1 CAPLUS
CN
     Benzeneethanol, β-[[6-[(3-chlorophenoxy)methyl]-2-phenyl-1H-
     pyrrolo[2,3/d]pyrimidin-4-yl]amino]-, (βS)- (9CI) (CA INDEX NAME)
Absolute stereochemistry.
10/035753
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RN
     343632-79-1 CAPLUS
CN
     Cyclopentanol, 3-[(2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]-, (3S)-
     (9CI)
           (CA INDEX NAME)
Absolute stereochemistry.
     343632-80-4 CAPLÚS
RN
     Acetamide, N-[2-\frac{1}{2}(2-pheny)]-6-[(2R)-2-[(phenylamino) methyl]-1-
CN
     pyrrolidinyl]methyl]-1H-pyrrolo[2,3-d]pyrimidin-4-yl]amino]ethyl]- (9CI)
     (CA INDEX NAME)
Absolute stereochemistry.
                         PhNH
    Ph
AcNH
RN
     343632/-81-5 CAPLUS
CN
     Benzeneethanol, \beta-[[6-[(3-chlorophenoxy)methyl]-2-phenyl-1H-
     pyrrolo[2,3-d]pyrimidin-4-yl]amino]-, (βR)- (9CI) (CA INDEX NAME)
Absolute stereochemistry.
```

10/035753

RN 343632-82-6 CAPLUS

CN 1-Piperidinecarboxamide, 2-[[[6-[(3-chlorophenoxy)methyl]-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl]amino]methyl]-N-methyl-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 343632-83-7 ¢APLUS

CN 1-Piperidinecarboxamide, 2-[[[6-[(3-chlorophenoxy)methyl]-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl]amino]methyl]-N-methyl-, (2R)- (9CI) (CA INDEX NAME) /

Absolute stereochemistry.

RN 343633-16-9 CAPLUS

Absolute stereochemistry.

RN 343969-97-1 CAPLUS

CN 1,2-Cyclopentanediol, 4-[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]-, $(1\alpha,2\alpha,4\beta)$ - (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 443118-58-9 CAPLUS

CN Benzeneethanol/ β -[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]-,/ (βS) - (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L4 ANSWER 8 OF 11 CAPLUS COPYRIGHT 2004 ACS on STN

AN 2002:368992 CAPLUS

DN 136:386128

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ΤI
     Synthesis and use of substituted pyrrolo[2,3-b]pyrimidines as selective
     adenosine A1, A2a and A3 receptor antagonists
     Castelhano, Arlindo L.; McKibben, Bryan; Witter, David J.
IN
PA
     OSI Pharmaceuticals, Inc., USA
     U.S. Pat. Appl. Publ/, 79 pp.
SO
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     MARPAT 136:386128
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Me
$$HN \rightarrow O$$
 $NH \rightarrow NH$ $R^4 \rightarrow R^3$ $R^2 \rightarrow NH$ $N \rightarrow NH$ $NH \rightarrow NH$ $NH \rightarrow NH$

Title compds. I and analogs [R2 = 5-6 membered aromatic ring; R3-4 = H, alkyl] were prepared Over 100 examples were provided. Intermediate 4-chloro-7H-pyrrolo[2,3-d]pyrimidines were prepared by several routes from appropriately substituted cyano-pyrroles. Thus, 4-chloro-2-(4-pyridyl)-7H-pyrrolo[2,3-d]pyrimidine hydrochloride was reacted with D-prolinol (2.3 mol equiv) in DMSO at 120°C for 18 h to yield II in 13% yield after purification Compound I [R2 = Ph; R3-4 = Me] exhibited 10-fold selectivity for binding to the adenosine A1 receptor than to A2a, A2b or A3 receptors. ClogP values were determined for selected example compds. I are useful for the treatment of COPD, allergic rhinitis, etc.

IT 246855-42-5P. Acetamide. N-[2-[(5.6-dimethyl-2-phenyl-1H-

246855-42-5P, Acetamide, N-[2-[(5,6-dimethyl-2-phenyl-1Hpyrrolo[2,3-d]pyrimidin-4-yl)amino]ethyl] - 251946-07-3P, Cyclopentanol, 3-[(5),6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4yl)amino]-,(1R,3R)-rel 251946-08-4P, Cyclopentanol, 3-[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]-,(1R,3S)rel 251946-09-5P 251946-37-9P, Acetamide, N-[2-[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]-1methylethyl] - 251946-38; OP, Acetamide, N-[(1R)-2-[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]-1-methylethyl]-251946-39-1P, Acetamide, N-[(2R)-2-[(5,6-dimethyl-2-phenyl-1Hpyrrolo [2, 3-d] pyrimidin $-4\frac{1}{2}$ yl) amino [2, 3-d] propyl [2, 3-d] pyrimidin $-4\frac{1}{2}$ yl) amino [2, 3-d] pyrimidin [2Acetamide, N-[(1S)-2-[(5,6]dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4yl)amino]-1-methylethyl]- 251946-41-5P, Acetamide, N-[(2S)-2-[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4yl)amino]propyl] - 251946-45-9P, Acetamide, N-[2-[(5,6-dimethyl-2phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]-1,1-dimethylethyl]-251946-46-0P, Acetamide, N-[2][(5,6-dimethyl-2-phenyl-1Hpyrrolo[2,3-d]pyrimidin-4-yl)amino[propyl] - 251946-52-8P, Glycine, (1R,3S)-3-[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4yl)amino]cyclopentyl ester, rel-, mono(trifluoroacetate)
251946-55-1P, Acetamide, N-[1-[[(5,6-dimethyl-2-phenyl-1Hpyrrolo[2,3-d]pyrimidin-4-yl)amino]methyl]propyl] - 343632-20-2P, Acetamide, N-[2-[(2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]ethyl]-343632-69-9P, 1H-Pyrrolo[2,3-d]pyrimidin-4-amine, 2-phenyl-N-[2-(1H-pyrrol-2-yl)ethyl] - 343632-77-9P, Cyclopentanol, 3-[(2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]-, (1S, 3R) - 343632-78-0P, Cyclopentanol, 3-[(2-phenyl-1Hpyrrolo[2,3-d]pyrimidin-4-yl) amino]-, (1R,3S)- 343632-79-1P, Cyclopentanol, 3-[(2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]-, (3S)-343632-80-4P, Acetamide, N-[2-[[2-phenyl-6-[[(2R)-2-[(phenylamino)methyl]-1-pyrrolidinyl]methyl]-1H-pyrrolo[2,3-d]pyrimidin-4yl]amino]ethyl] - 343632-81-5p, Benzeneethanol,

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β-[[6-[(3-chlorophenoxy)methyl]-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-
             yl]amino]-, (βR)- 343632-82-6P, 1-Piperidinecarboxamide,
             2-[[[6-[(3-chlorophenoxy)methyl]/2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-
             yl]amino]methyl]-N-methyl-, (25)- 343632-83-7P,
             1-Piperidinecarboxamide, 2- [√[6-[(3-chlorophenoxy)methyl]-2-phenyl-1H-
             pyrrolo[2,3-d]pyrimidin-4-x1]amino]methyl]-N-methyl-, (2R)-
             343633-16-9P, Cyclopentapol, 3-[(2-phenyl-1H-pyrrolo[2,3-
             d]pyrimidin-4-yl)amino]\neq, (1S,3S)- 343969-97-1P,
             1,2-Cyclopentanediol, /4-[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-
             4-y1) amino] -, (1\alpha, 2\alpha, 4\beta)
             RL: BSU (Biological/study, unclassified); PAC (Pharmacological activity);
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             study); PREP (Preparation); USES (Uses)
                     (preparation and use of substituted 7H-pyrrolo[2,3-b]pyrimidines as
                    selective ademosine A1, A2a and A3 receptor antagonists)
RN
             246855-42-5 CAPLUS
            Acetamide, N-[2/[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-
CN
            yl)amino]ethyl]/- (9CI)
                                                                      (CA INDEX NAME)
                                                              Me
                                                            Me
ACNH-CH2-CH2-NH
RN
            251946-07-3 CAPLUS
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CN
            yl)amino]-, (1R,3R)-rel- (9CI) (CA INDEX NAME)
Relative stereochemistry.
                                                              Me
RN
            251946-08-4 CAPLUS
            Cyclopentanol, 3-[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-
CN
            yl)amino]-, (1R,3S)-rel/- (9CI) (CA INDEX NAME)
Relative stereochemistry.
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RN 251946-09-5 CAPLUS

CN 1,2-Cyclopentanediol, 4-[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]-/stereoisomer (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 251946-37-9 CAPLUS

CN Acetamide, N-[2-\[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]-1-methylethyl]- (9CI) (CA INDEX NAME)

RN 251946-38-0 CAPLUS

CN Acetamide, N-[(1R)-2-[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]-1-methylethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry

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RN 251946-39-1 CAPLUS
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CN Acetamide, N-[(2R)-2-[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]propyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 251946-40-4 CAPLUS

CN Acetamide, N-[(1S)/2-[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]-1-methylethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 251946-41-5 CAPLUS

CN Acetamide, N-[(2S)-2-[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]propyl] (9CI) (CA INDEX NAME)

Absolute stereochemistky.

RN 251946-45-9 CAPLUS

CN Acetamide, N-[2-[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]-1,1-dimethylethyl]- (9CI) (CA INDEX NAME)

Мe Ph. AcNH Мe $Me-C-CH_2-NH$ Мe RN251946-46-0 CAPLUŞ CNAcetamide, N-[2-[/5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4yl)amino]propyl]-/ (9CI) (CA INDEX NAME) Ph Мe Me Acnh-CH2-CH-NH Мe RN251946-52-8 CAPLUS CNGlycine, (1R,3S)-3-[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4yl)amino]cyclopentyl ester, rel-, mono(trifluoroacetate) (9CI) (CA INDEX NAME) CM 1 CRN 251946-51-7 CMF C21 H25 N5 O2 Relative stereochemistry Me Me NH Ph CM 2

CRN

CMF

76-05-1

C2 H F3 O2

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CO2H
RN
      251946-55-1 CAPLUS
     Acetamide, N-[1-[[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-
CN
     yl)amino]methyl]propyl]-/(9CI) (CA INDEX NAME)
                        Me
    NHAc
Et-CH-CH2-NH
RN
     343632-20-2 CAPLUS
CN
     Acetamide, N-[2-[(2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]ethyl]-
            (CA INDÉX NAME)
Acnh-CH2-CH2-NH
RN
     343632-69-9 CAPLUS
CN
     1H-Pyrrolo[2,3-d]pyrimidin-4-amine, 2-phenyl-N-[2-(1H-pyrrol-2-yl)ethyl]-
      (9CI) (CA INDEX\NAME)
       CH<sub>2</sub>
       CH<sub>2</sub>
       NH
Ph
RN
     343632-77-9 CAPLUS
     Cyclopentanol, 3-[(2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]-, (1S,3R)- (9CI) (CA INDEX NAME)
CN
Absolute stereochemistry.
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RN
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     Cyclopentanol, 3-[(2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]-,
CN
                     (CA INDEX NAME)
     (1R,3S) - (9CI)
Absolute stereochemistry
              NH
RN
     343632-79-1 CAPLUS
     Cyclopentanol, 3-1[(2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]-, (3S)-(9CI) (CA INDEX NAME)
CN
Absolute stereochemistry.
RN
     343632-80-4 CAPLÚS
     Acetamide, N-[2-[12-phenyl-6-[[(2R)-2-[(phenylamino)methyl]-1-
CN
     pyrrolidinyl]methyl]-1H-pyrrolo[2,3-d]pyrimidin-4-yl]amino]ethyl]- (9CI)
     (CA INDEX NAME)
Absolute stereochemistry.
```

CN Benzeneethanol, β -[[6-[(3-chlorophenoxy)methyl]-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl]amino]-, (β R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 343632-82-6 CAPLUS

CN 1-Piperidinecarboxamide, 2-[[[6-[(3-chlorophenoxy)methyl]-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl]amino]methyl]-N-methyl-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 343632-83-7 CAPLUS

CN 1-Piperidinecarboxamide, 2-[[[6-[(3-chlorophenoxy)methyl]-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl]amino]methyl]-N-methyl-, (2R)- (9CI) (CA INDEX NAME)

10/035753

Absolute stereochemistry.

RN 343633-16-9 CAPLUS

CN Cyclopentanol, 3-[(2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]-, (1S,3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 343969-97-1 CAPLUS

CN 1,2-Cyclopentanediol, 4-[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]-, $(1\alpha,2\alpha,4\beta)$ - (9CI) (CA INDEX NAME)

Relative stereochemistry

L4 ANSWER 9 OF 11 CAPLUS COPYRIGHT 2004 ACS on STN

AN 2001:416773 CAPLUS

DN 135:46190

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ΤI
     Synthesis and use of substituted pyrrolo[2,3-b]pyrimidines as selective
     adenosine A1, A2a and A3 receptor antagonists
IN
     Castelhano, Arlindo L.; McKibben, Bryan; Witter, David J.
     Osi Pharmaceuticals, Inc., USA
PA
so
     PCT Int. Appl., 368 pp.
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os
GI
                                                  OH
             R5
                     I
                                                       III
AB
     The synthesis of compds. I, their binding to adenosine receptors and use
     are described [wherein; R1, R2 = H, (un) substituted alkyl or NR1R2 = (un) substituted 4-8 membered ring; R3 = (un) substituted 4-6 membered
     (aromatic) ring; R4, R5 = H, (un) substituted alkyl, aryl (with some
     exceptions)]. Over 100 examples are provided. Intermediate
     4-chloro-7H-pyrrolo[2,3-d]pyrimidines were prepared by several routes from
     appropriately substituted cyano-pyrtoles. Thus, 4-chloro-2-(4-pyridyl)-7H-
     pyrrolo[2,3-d]pyrimidine hydrochloride was reacted with D-prolinol (2.3
     mol equiv) in DMSO at 120°C for 18 /h to yield III in 13% yield
     after purification Compound I [R1/= AcNHCH2CH2; R2 = H; R3 = Ph; R4, R5 = Me;
     II] exhibited selective binding to adenosine receptor A1 with IC50 = 82.8
     nM. Compound II also had Ki = 9.8 nM (vs. Ki = 7.1 for control ligand 8-cyclopentyl-1,3-dipropylxanthine (DPCPX)). Pyrimidine III binds 5 times
```

more selectively to adenosine receptor A2a than A1, A2b or A3 (no data). Compound I [R1 = AcNH(CH2)4; R2 = H; R3 = Ph; R4, R5 = Me] is 10 times more selective for A3 than the other receptor subtypes. ClogP (calculated partition coefficient between octanol and H2O) values were determined for

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selected

example compds. Claimed uses of I includes administration of a systemic formulation (i.e. ophthalmic) for the treatment of a disease associated with A1, A2a, and A3 adenosine receptors in a subject. IT 246855-42-5P 251946-07-3P 251946-08-4P 251946-09-5P 251946-37-9P 251946-38-0P 251946-39-1P 251946-40-4P 251946-41-5P 251946-45-9P 251946-46-0P 251946-52-8P 251946-55-1P 343632-20-2P/343632-31-5P 343632-32-6P 343632-33-7/P 343632-35-9P 343632-36-0P 343632-37-1P 343632-38-2P 343632-39-3P 343632-40/-6P 343632-41-7P 343632-43-9P 343632-44-0P 343632-45-1P 343632-46-2P 343632-69-9P 343632-77-9P 343632-78-0P 343632-/79-1P 343632-80-4P 343632-81-5P 343632-82-6P 343632-83-7P 343633-16-9P 343969/97-1P RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses) (preparation and use of substituted 7H-pyrrolo[2,3-b]pyrimidines as selective adenosine A1, A2a and A3 receptor antagonists) RN 246855-42-5 CAPLUS Acetamide, N-[2-[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-CN yl)amino]ethyl]- (9CI) (CA INDEX NAME) Me ACNH-CH2-CH2-NH 251946-07-3 CAPLUS RN CN Cyclopentanol, 3-[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4yl)amino]-, (1R,3R)-rel- (9CI) (CA INDEX NAME) Relative stereochemistry. Me 251946-08-4 CAPLUS ВN Cyclopentanol / 3-[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-CNyl)amino]-, (1R,3S)-rel- (9CI) (CA INDEX NAME) Relative stereochemistry.

RN 251946-09-5 CAPLUS

CN 1,2-Cyclopentanediol, 4-[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]-, stereoisomer (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 251946-37-9 \CAPLUS

CN Acetamide, N-[2-[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]-1-methylethyl]- (9CI) (CA INDEX NAME)

RN 251946-38-0 CAPLUS

CN Acetamide, N-[(1R)-2-[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]-1-methylethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

10/035753

RN 251946-39-1 CAPLUS

CN Acetamide, N-[(2R)-2-[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]propyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 251946-40-4 CAPLUS

CN Acetamide, N-[(1S)-2-[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]-1-methylethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 251946-41-5 CAPLUS

CN Acetamide, N-[(2S) \2-[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]propyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry

RN 251946-45-9 CÁPLUS

CN Acetamide, $N-\sqrt{2-[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]-1,1-dimethylethyl]- (9CI) (CA INDEX NAME)$

Me

NH

Ph

CM

CRN

CMF

2

76-05-1

C2 H F3 O2

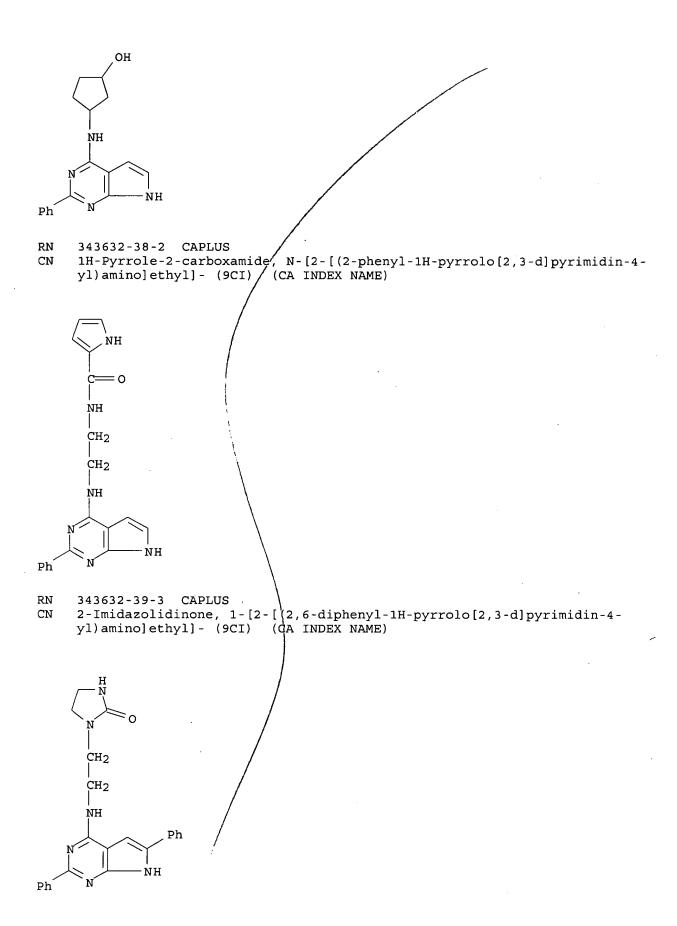
 $Et_2N-C-NH-CH_2-CH_2-NH$

RN 343632-33-7 CAPLUS Ethanethioamide, N-[2-[(5,6-dimethyl-2-pheny]'-1H-pyrrolo[2,3-d]pyrimidin-4CNyl)amino]ethyl]- (9CI) (CA INDEX NAME) Me Me $Me-C-NH-CH_2-CH_2-NH$ 343632-35-9 CAPLUS RNUrea, N-[3-[(5,6-dimeth/1-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-CNyl)amino]propyl]-N'-ethyl- (9CI) (CA INDEX NAME) Me Me EtNH-C-NH- $(CH_2)_3$ -NH RN343632-36-0 CAPLUS Glycine, 3-[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-CNyl)amino]cyclopentyl ester (9CI) (CA INDEX NAME) H_2N-CH_2 NH Me Me Ph RN 343632-37-1 CAPLUS

Cyclopentanol / 3-[(2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]- (9CI)

CN

(CA INDEX NAME)



343632-40-6 CAPLUS CN Butanamide, 2-[(2,6-diphenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]-3methyl- (9CI) (CA INDEX NAME) H2Ni-Pr-CH-NH RN 343632-41-7 CAPLUS Benzenepropanamide, CN α -[(2,6-diphenyl-1H-pyrrolo[2,3-d]pyrimidin-4yl)amino] - (9CI) CA INDEX NAME) CH2-Ph H2N-C-- CH-- NH Ph RN343632-43-9 CAPLUS 1H-Pyrrolo[2,3-d]pyrimidin-4-amine, 6-[(3-chlorophenoxy)methyl]-2-phenyl-N-CN . [2-(1H-pyrrol-2-yl)ethyl] (9CI) (CA INDEX NAME) CH₂CH₂ NH Ph RN343632-44-0 CAPLUS CN Acetamide, N-[2-[[2-phenyl-6-[[(2S)-2-[(phenylamino)methyl]-1pyrrolidinyl]methyl]-fH-pyrrolo[2,3-d]pyrimidin-4-yl]amino]ethyl]- (9CI) (CA INDEX NAME) Absolute stereochemistry

CN Benzeneethanol, β-[[6-[(3-chlorophenoxy)methyl]-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4/yl]amino]-, (βS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 343632-46-2 CAPLUS

CN 1-Piperidinecarboxamide, 2-[[[6-[(3-chlorophenoxy)methyl]-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl]amino]methyl]-N-methyl- (9CI) (CA INDEX NAME)

RN 343632-69-9 CAPLUS

CN 1H-Pyrrolo[2,3-d/pyrimidin-4-amine, 2-phenyl-N-[2-(1H-pyrrol-2-yl)ethyl]-(9CI) (CA INDEX NAME)

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CH<sub>2</sub>
       CH<sub>2</sub>
       ŅН
Ph
RN
     343632-77-9 CAPLUS
     Cyclopentanol, 3-[(2-phen/1-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]-,
CN
      (1S, 3R) - (9CI)
                     (CA INDEX NAME)
Absolute stereochemistry.
RN
     343632-78-0 CAPLUS
     Cyclopentanol, 3-[(2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]-,
CN
     (1R,3S) - (9CI) (CA INDEX NAME)
Absolute stereochemistry.
RN
     343632-79-1 CAPLUS
CN
     Cyclopentanol, 3-[(2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]-, (3S)-
           (CA INDEX NAME/)
     (9CI)
Absolute stereochemistry
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Absolute stereochemistry.

INDEX NAME)

CN 1-Piperidinecarboxamide, 2-[[[6-[(3-chlorophenoxy)methyl]-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl]amino]methyl]-N-methyl-, (2R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 343633-16-9 CAPLUS

CN Cyclopentanol, 3-[(2-phenyl-1H-pyrrplo[2,3-d]pyrimidin-4-yl)amino]-, (1S,3S)- (9CI) (CA INDEX NAME)

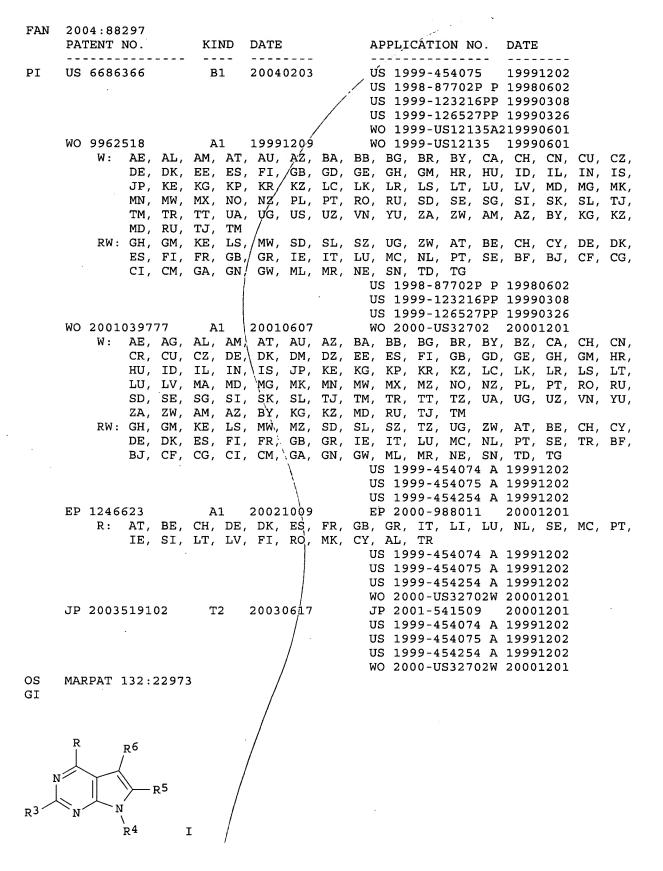
Absolute stereochemistry.

RN 343969-97-1 CAPLUS

CN 1,2-Cyclopentanediol, 4-[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]-, $(1\alpha,2\alpha,4\beta)$ - (9CI) (CA INDEX NAME)

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RE.CNT 1
              THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD
              ALL CITATIONS AVAILABLE IN THE RE FORMAT
L4
     ANSWER 10 OF 11 CAPLUS COPYRIGHT 2004 ACS on STN
     1999:783937 CAPLUS
AN
     132:22973
DN
     Preparation of pyrrolo[2,3-d]pyrimidines as adenosine receptor antagonists
ΤI
     Castelhano, Arlindo L.\; McKibben, Bryan; Witter, David J.
IN
PA
     Cadus Pharmaceutical Corp., USA
so
     PCT Int. Appl., 169 pp.
     CODEN: PIXXD2
DT
     Patent
     English
LA
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     PATENT NO.
                      KIND DATE
                                           APPLICATION NO. DATE
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             BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG
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                                           US 1999-454254 A 19991202
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AB Title compds. [I; R = NR1R2; R1-R4 = H, alkyl, aryl, etc.; NR1R2 =

heterocyclyl; R5,R6 = H, halo, alkyl, aryl, etc.; R4R5,R5R6 = atoms to complete a ring] were prepared Thus, 2- amino-3-cyano-4,5-dimethyl-1-(1-phenylethyl)pyrrole was N-benzoylated and the product cyclized to give, after deprotection and chlorination, I (R3 = Ph, R4 = H, R5 = R6 = Me)(II; R = Cl) which was aminated by trans-4-hydroxycyclohexylamine to give II (R = trans-4-hydroxycyclohexylamino). Data for biol. activity of I were given.

IT 246855-42-5P 251946-07-3P 251946-08-4P 251946-09-5P 251946-37-9P 251946-38-0P 251946-39-IP 251946-40-4P 251946-41-5P 251946-45-9P 251946-46-0P 251946-52-8P 251946-55-IP
RL: BAC (Biological activity or effector, except adverse); BSU (Biological

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of pyrrolo[2,3-d]pyrimidines as adenosine receptor antagonists)

RN 246855-42-5 CAPLUS CN Acetamide. N-[2-/[(5

Acetamide, N-[2-[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]ethyl] (9CI) (CA INDEX NAME)

AcNH-CH2-CH2-NH

RN 251946-07-3 CAPLUS

CN Cyclopentanol, 3-[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]-, (1R,3R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 251946-08-4 CAPLUS

CN Cyclopentanol, 3-[(5/,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]-, (1R,3S)/rel- (9CI) (CA INDEX NAME)

Relative stereochemistry

RN 251946-09-5 CAPLUS

CN 1,2-Cyclopentanediol, 4-[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]-, stereoisomer (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 251946-37-9 \ CAPLUS

CN Acetamide, N_{1}^{1} [2-[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]-1-methylethyl]- (9CI) (CA INDEX NAME)

RN 251946-38-0 CAPLUS

CN Acetamide, N-[/(1R)-2-[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]-1-methylethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 251946-39-1 CAPLUS

CN Acetamide, N-[(2R)-2-[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]propyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 251946-40-4 CAPLUS

CN Acetamide, N-[(1 \dot{S})-2-[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]-1-methylethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 251946-41-5 CAPLUS

CN Acetamide, N-[(2S)-2-[\(5,6-\)dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]propyl]- (9CI)\((CA INDEX NAME)

Absolute stereochemistry.

RN 251946-45-9 CAPLUS

CN Acetamide, N-[2-[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]-1,1-dimethylethyl]- (9CI) (CA INDEX NAME)

RN 251946-46-0 CAPLUS

CN Acetamide, N-[2-[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]propyl]- (9CI)/ (CA INDEX NAME)

RN 251946-52-8 CAPLUS

CN Glycine, (1R,3S)-3-[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]cyclopentyl ester, rel-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 251946-51-7 CMF C21 H25 N5 O2

Relative stereochemistry.

RN 251946-55-1 CAPLUS

CN Acetamide, N-[1-[[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]methyl]propyl]- (9CI) (CA INDEX NAME)

RE.CNT 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 11 OF 11 CAPLUS COPYRIGHT 2004 ACS on STN

AN 1999:571295 CAPLUS

DN 131:281026

TI Selective A1-adenosine receptor antagonists identified using yeast Saccharomyces cerevisiae functional assays

AU Campbell, Robert M.; Cartwright, Craig; Chen, Wei; Chen, Yong; Duzic, Emir; Fu, Jian-Min; Loveland, Michelle; Manning, Ron; McKibben, Bryan; Pleiman, Christopher M.; Silverman, Lauren; Trueheart, Joshua; Webb, David R.; Wilkinson, Vicki; Witter, David J.; Xie, Xiaobing; Castelhano, Arlindo I.

CS Cadus Pharmaceutical Corporation, Tarrytown, NY, 10591, USA

SO Bioorganic & Medicinal Chemistry Letters (1999), 9(16), 2413-2418 CODEN: BMCLE8; ISSN: 0960-894X

PB Elsevier Science Ltd.

DT Journal

LA English

I

AB Evaluation of a biased "library" of pyrrolo[2,3-d]pyrimidines using yeast-based functional assays expressing human A1- and A2a-adenosine receptors, led to the A1 selective antagonist I. A direct correlation

10/035753

between yeast functional activity and binding data was established. Practical compds. with polar residues at C-4 of the pyrrolopyrimidine system required H-bond donor functionality for high potency.

IT 246855-42-5P 246855-48-1P

RL: BPR (Biological process); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); PROC (Process)

(selective A1-adenosine receptor antagonists identified using yeast functional assays)

RN 246855-42-5 CAPLUS

CN Acetamide, N-[2-[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]ethyl]- (9CI) (CA INDEX NAME)

 $Acnh-Ch_2-Ch_2-Nh$

RN 246855-48-1 CAPLUS

CN 2-Imidazolidinone, 1-[2-[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]ethyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & H & \\ & N & \\ & & \\ & CH_2 & \\ & CH_2 & \\ & & \\ & CH_2 & \\ & & \\ & NH & Me & \\ & & \\ & NH & Me & \\ & & \\ & NH & Me & \\ & & \\ & NH & Me & \\ & & \\ & NH & Me & \\ & & \\ & NH & Me & \\ & & \\ & NH & Me & \\ & & \\ & NH & Me & \\ & & \\ & NH & Me & \\ & & \\ & NH & Me & \\ & & \\ & NH & Me & \\ & & \\ & NH & Me & \\ & & \\ & NH & Me & \\ & \\ & NH & \\ &$$

RE.CNT 18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT